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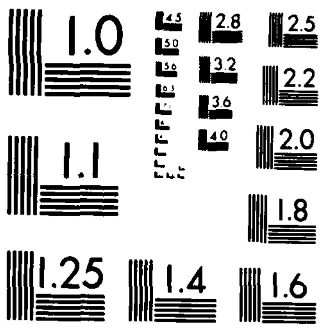

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ON THE CHARACTERIZATION OF NONNEGATIVELY ESTIMABLE LINEAR COMBINATIONS OF VARIANCE COMPONENTS

by

Thomas Mathew*

Center for Multivariate Analysis

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March 1984

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ON THE CHARACTERIZATION OF NONNEGATIVELY ESTIMABLE LINEAR COMBINATIONS OF VARIANCE COMPONENTS

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Abbreviated Title: NONNEGATIVE ESTIMABILITY

Summary

It is ~~shown~~ that, by a reparametrization, the problem of estimating a linear combination of variance components can be reduced to that of estimating a single variance component. Such a reduction is used to obtain some characterizations of nonnegatively estimable linear combinations of variance components. Characterization of nonnegative estimability using MINQUE is also discussed.

*On leave from Indian Statistical Institute.

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Key words and phrases. Nonnegative estimability. MINQUE (given Σ), MINQUE (Σ,NND), quadratic subspace, subspaces that preserve nonnegative definiteness.

1. Introduction. Recently, much attention has been given to the problem of nonnegative estimation of variance components. Several nonnegative estimators have been proposed sacrificing unbiasedness; see e.g., P.S.R.S. Rao and Chaubey (1978), Hartung (1981) and Chaubey (1983). In the works of LaMotte (1973), Pukelsheim (1981a,b), Mathew (1984) and Baksalary and Molinska (1984), the main concern is the existence of nonnegative definite (nnd) quadratic estimators that are also unbiased. The present work is concerned with the existence and characterization of nnd quadratic unbiased estimators (QUE's) of a linear combination of variance covariance components.

The problem of nonnegative estimation of variance components is not fully resolved by characterizing linear combinations of variance components that admit nnd QUE's. It should also be possible to obtain an nnd QUE having some optimal properties (for e.g. properties similar to those of C.R. Rao's MINQUE). The work of Pukelsheim (1981a) is a significant achievement in this regard. Under a quadratic subspace condition, Pukelsheim showed that in order to verify nonnegative estimability, it is enough to check the nonnegativity of the MINQUE (given I). This actually solves the problem of nonnegative estimability of variance components from balanced data, since, as observed by Anderson, et. al. (1984 p. 170), the quadratic subspace condition is always satisfied in this case. Pukelsheim's result has been extended by Mathew (1984). However, the procedure outlined in Pukelsheim (1981a) and Mathew (1984) will not always work for unbalanced data.

In the next section we show that, by a suitable reparametrization, the problem of estimating a linear combination of variance components can be reduced to that of estimating a single variance component. This reduction has enabled us to obtain some characterizations of nonnegatively estimable linear combinations of variance components and also to obtain nnd QUE's. A complete solution is given to the nonnegative estimation problem in the case of a model with two

variance components. These are discussed in section 3. In section 4 we consider the problem of characterizing nonnegative estimability using MINQUE.

2. Notations and Preliminary Results.

Let Y be a random R^n-vector with $E(Y) = X\beta$ and $D(Y) = V_\theta = \sum_{i=1}^{k} \theta_i V_i$. Here X is a known $n\times m$ $(m<n)$ matrix, β is a vector of unknown parameters varying over R^m, $V_i (i = 1,2,\ldots,k)$ are known real symmetric matrices and $\theta = (\theta_1,\theta_2,\ldots,\theta_k)'$ is a vector of unknown parameters varying over the set Θ, a subset of R^k. The following assumptions are made regarding the matrix V_θ and the set Θ

(i) for each $\theta \in \Theta$, V_θ is nnd (1)

(ii) the elements of Θ span R^k (2)

(iii) there exists an nnd matrix $V_o \in SP\{V_\theta\colon \theta \in \Theta\}$ such that for $i = 1,2,\ldots,k$ $\mathcal{R}(V_i) \subset \mathcal{R}(V_o)$ (3)

Here $\mathcal{R}(\cdot)$ denotes range. We denote the above model as

$$Y \sim (X\beta,\ V_\theta), \qquad \theta \in \Theta \tag{I}$$

The unknown θ_i's could be components of variance or covariance. We are interested in estimating a linear combination $q'\theta = q_1\theta_1 + q_2\theta_2 + \ldots + q_k\theta_k$, the estimators under consideration being quadratic forms in Y. We assume without loss of generality that $q'q = 1$ and $q_k \neq 0$. For an $n\times n$ positive definite (p.d.) matrix Σ, let $M_\Sigma = I - X(X'\Sigma^{-1}X)^- X'\Sigma^{-1}$ (A^- denotes a generalized inverse of the matrix A) and let S_Σ be the matrix whose $(ij)^{th}$ element is tr $\Sigma^{-1}M_\Sigma V_i M_\Sigma' \Sigma^{-1} V_j$ $(i,j = 1,2,\ldots,k)$. Then it can be shown that $\mathcal{R}(S_\Sigma)$ does not depend on Σ and $q'\theta$ has an invariant quadratic unibased estimator (IQUE) iff $q \in \mathcal{R}(S_\Sigma)$. When $q \in \mathcal{R}(S_\Sigma)$, the MINQUE (given Σ) of $q'\theta$ is given by $Y'(\sum_{j=1}^{k} \lambda_j \Sigma^{-1} M_\Sigma V_j M_\Sigma' \Sigma^{-1})Y$, where $\lambda = (\lambda_1,\ldots,\lambda_k)'$ is

any solution to $S_{\Sigma}\lambda = q$. The MINQUE (given Σ) of $q'\theta$ is the unique estimator obtained by minimizing tr $A\Sigma A\Sigma$, where A is any symmetric matrix satisfying the conditions $AX = 0$ and tr $AV_i = q_i$ $(i = 1,2,\ldots,k)$. For the details, we refer to Rao (1970, 1971, 1972, 1973), Kleffe (1977) or Rao and Kleffe (1980). For our discussion, it is conveneint to have the following definitions. Definition 1 is due to Pukelsheim (1981a).

Definition 1 We say that $q'\theta$ is nonnegatively estimable in model (I) if it has a nonnegative definite quadratic unbiased estimator.

Definition 2 We say that MINQUE (given Σ) characterizes nonnegative estimability in model (I) if, for every vector $q \in R^k$, the nonnegative estimability of $q'\theta$ implies the nonnegativity of its MINQUE (given Σ).

For a nonnegatively estimable $q'\theta$ and for a p.d. Σ, let B_* minimize tr $B\Sigma B\Sigma$, where B is any nnd matrix such that $Y'BY$ is an unbiased estimator of $q'\theta$. We shall refer to $Y'B_*Y$ as the MINQUE (Σ, NND) of $q'\theta$. Let

$$Q = \begin{bmatrix} 1-q_1^2 & -q_1q_2 & -q_1q_3 & \cdots\cdots & -q_1q_{k-1} & q_1 \\ -q_2q_1 & 1-q_2^2 & -q_2q_3 & \cdots\cdots & -q_2q_{k-1} & q_2 \\ \hline -q_{k-1}q_1 & -q_{k-1}q_2 & -q_{k-1}q_3 & \cdots\cdots & 1-q_{k-1}^2 & q_{k-1} \\ -q_kq_1 & -q_kq_2 & -q_kq_3 & \cdots\cdots & -q_kq_{k-1} & q_k \end{bmatrix} .$$

Then $|Q| = q_k$, which is nonzero (by our assumptions $q'q = 1$ and $q_k \neq 0$). For $\eta = (\eta_1,\eta_2,\ldots,\eta_k)'$, if we let $\theta = Q\eta$, then $\theta_1V_1+\theta_2V_2+\ldots+\theta_kV_k = \eta_1(V_1-q_1V_q) + \eta_2(V_2-q_2V_q)+\ldots+\eta_{k-1}(V_{k-1}-q_{k-1}V_q) + \eta_kV_q$. Here $V_q = \sum_{i=1}^{k} q_iV_i$. We now consider the model

$$Y \sim (X\beta,\ \sum_{i=1}^{k-1} \eta_i(V_i - q_i V_q) + \eta_k V_q) \qquad \text{(II)}$$

where $\eta \in Q^{-1}\Theta = \{Q^{-1}\theta: \theta \in \Theta\}$.

Lemma 1 (i) Every QUE (or IQUE) of $q'\theta$ in model (I) is a QUE (respectively IQUE) of η_k in model (II) and vice versa.

(ii) The nonnegative estimability of $q'\theta$ in (I) is equivalent to the nonnegative estimability of η_k in (II).

(iii) For any p.d. Σ, the MINQUE (given Σ) of $q'\theta$ in (I) is same as the MINQUE (given Σ) of η_k in (II).

(iv) If $q'\theta$ is nonnegatively estimable in (I), then for any p.d. Σ, the MINQUE (Σ, NND) of $q'\theta$ in (I) is same as the MINQUE (Σ, NND) of η_k in (II).

Proof: $Y'AY$ is a QUE (or IQUE) of $q'\theta$ in (I) iff $\operatorname{tr} AV_i = q_i$ $(i = 1,2,\ldots,k)$ and $X'AX = 0$ (respectively $AX = 0$). Then $\operatorname{tr} AV_q = \Sigma q_i^2 = 1$ (by assumption). Since $V_k - q_k V_q = -\frac{1}{q_k}\sum_{i=1}^{k-1} q_i(V_i - q_i V_q)$, the condition $\operatorname{tr} AV_i = q_i$ $(i = 1,2,\ldots,k)$ is seen to be equivalent to the conditions $\operatorname{tr} AV_q = 1$ and $\operatorname{tr} A(V_i - q_i V_q) = 0$ $(i = 1,2,\ldots,k-1)$. This proves the assertion in (i). (ii) follows from (i). Since the class of IQUE's of $q'\theta$ in (I) and η_k in (II) are the same, the minimum norm element in this class gives the MINQUE (given Σ) of $q'\theta$ as well as η_k. This proves part (iii). (iv) follows similarly. □

3. Nonnegative Estimation.

When the matrices V_i $(i = 1,2,\ldots,k)$ are nnd, conditions for the nonnegative estimability of a single variance component in the model (I) has been derived by Pukelsheim (1977, Theorem 5.1). Alternativeforms of the same condition are given in Kleffe (1977, Theorem 3) and Rao and Kleffe (1980, Theorem 5.5.1). We now proceed to obtain similar results for the nonnegative estimability of $q'\theta$.

The following lemma will be used in the sequel. When a symmetric matrix A is nnd, we denote $A \geq 0$.

Lemma 2 (Pukelsheim, 1981a). Let $M = I-XX^+$. Then $q'\theta$ is nonnegatively estimable in (I) iff $t_1MV_1M+\ldots+t_kMV_kM \geq 0$ implies $q_1t_1+\ldots+q_kt_k \geq 0$.

Let P_q denote the orthogonal projector onto the subspace $R(MV_1M-q_1MV_qM)+\ldots+R(MV_{k-1}M-q_{k-1}MV_qM)$, i.e. if the columns of the matrix H form a basis for this subspace, then $P_q = H(H'H)^{-1}H'$. Further, let $V_M(q)$ denote the vector space spanned by the matrices $M(V_i-q_iV_q)M$ $(i = 1,2,\ldots,k-1)$.

Theorem 1. (i) If $(I-P_q)MV_qM(I-P_q)$ is non-null, then $q'\theta$ is nonnegatively estimable in (I) iff $(I-P_q)MV_qM(I-P_q)$ is nnd.

(ii) If there exists an nnd matrix $W_0 \in V_M(q)$ satisfying $R(MV_iM-q_iMV_qM) \subset R(W_0)$ for $i = 1,2,\ldots,k-1$, then $q'\theta$ is nonnegatively estimable in (I) iff $(I-P_q)MV_qM(I-P_q)$ is nonnull and nnd.

Proof: Let

$$\begin{aligned} U_i &= V_i-q_iV_q \quad \text{for } i = 1,2,\ldots,k-1 \\ &= V_q \quad \text{for } i = k. \end{aligned}$$

From Lemma 2 and Lemma 1 (ii), it follows that $q'\theta$ is nonnegatively estimable in (I) iff $t_1MU_1M+\ldots+t_kMU_kM \geq 0 \Rightarrow t_k \geq 0$, where $M = I-XX^+$. In view of assumption (2) about Θ, there exists a nonnull t_k satisfying $t_1MU_1M+\ldots+t_kMU_kM \geq 0$. This implies $t_k(I-P_q)MV_qM(I-P_q) \geq 0$. If $(I-P_q)MV_qM(I-P_q)$ is a nonnull matrix, since t_k is nonnull, t_k is positive iff $(I-P_q)MV_qM(I-P_q)$ is nnd. This proves part (i). The "if" part in (ii) is clear from (i). The "only if" part also follows from (i) once it is shown that for $q'\theta$ to be nonnegatively estimable, $(I-P_q)MV_qM(I-P_q)$ must be nonnull when there exists a matrix W_0 as specified in the theorem. Suppose $(I-P_q)MV_qM(I-P_q) = 0$. Let $\sum_{i=1}^{k} t_iMU_iM > 0$ where

$t_k \neq 0$. Since $P_q MU_iM = MU_iM$ for $i = 1,2,\ldots,k-1$, $\sum_{i=1}^{k} t_iMU_iM \geq 0$ can equivalently be written as $P_q(\sum_{i=1}^{k-1} MU_iM)P_q + t_k[(I-P_q)MV_qMP_q + P_qMV_qM(I-P_q) + P_qMV_qMP_q] \geq 0$. This gives $(I-P_q)MV_qMP_q = 0$, which, along with $(I-P_q)MV_qM(I-P_q) = 0$ yields $(I-P_q)MV_qM = 0$ or equivalently $R(MV_qM) \subset R(W_0)$ and hence there exists $t_k < 0$ such that $W_0 + t_kMV_qM \geq 0$. This contradicts the nonnegative estimability of $q'\theta$ since W_0 is a linear combination of MU_iM $(i = 1,2,\ldots,k-1)$. □

Remark 1 If $(I-P_q)MV_qM(I-P_q)$ is nonnull, then it cannot be indefinite. From the proof of Theorem 1 it follows that there exists $t_k \neq 0$ satisfying $t_k(I-P_q)MV_qM(I-P_q) \geq 0$. Hence $(I-P_q)MV_qM(I-P_q)$ is either nnd or nonpositive definite. In case it is nonpostive definite, $q'\theta$ has a nonpositive definite quadratic unbiased estimator.

In the case of a model with two variance components, the following corollary gives a complete characterization of nonnegatively estimable $q'\theta$.

Corollary 1. Suppose $k = 2$ in model (I). Let P_q and M be as defined before.

(i) If $(I-P_q)MV_qM(I-P_q)$ is nonnull, then $q'\theta$ is nonnegatively estimable iff $(I-P_q)MV_qM(I-P_q)$ is nnd.

(ii) If $MV_1M-q_1MV_qM$ is nnd or nonpositive definite, then $q'\theta$ is nonnegatively estimable iff $(I-P_q)MV_qM(I-P_q)$ is nonnull and nnd.

(iii) If $MV_1M-q_1MV_qM$ is indefinite and if $(I-P_q)MV_qM(I-P_q) = 0$, then $q'\theta$ is nonnegatively estimable iff (a) $R(MV_qM) \subset R(MV_1M-q_1MV_qM)$ and (b) there exists a real number α such that $MV_qM+\alpha(MV_1M-q_1MV_qM)$ is nnd.

Proof: Only part (iii) needs to be proved. Suppose $q'\theta$ is nonnegatively estimable. If $(I-P_q)MV_qM(I-P_q) = 0$, then proceeding as in the proof of Theorem 1 (ii), we get $R(MV_qM) \subset R(MV_1M-q_1MV_qM)$. Since there exists a nonnull real

number t_2 satisfying $t_1(MV_1M-q_1MV_qM)+t_2MV_qM \geq 0$, the nonnegative estimability of $q'\theta$ demands that there exists a positive t_2 satisfying the same, which leads to part (b). To prove the sufficiency of the conditions, we observe that since $MV_1M-q_1MV_qM$ is indefinite, conditions (a) and (b) guarantee the existence of an nnd matrix A satisfying tr $A(MV_1M-q_1MV_qM)=0$ and tr $A(MV_qM+\alpha(MV_1M-q_1MV_qM))>0$ or equivalently tr $AMV_qM > 0$. Then $\frac{1}{\text{tr } AMV_qM} Y'MAMY$ is an nnd unbiased estimator of $q'\theta$. □

In the case of a model with two variance components with V_1,V_2 nnd, we shall now obtain explicit characterization of vectors q for which $q'\theta$ is nonnegatively estimable. To this end, let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r$ denote the proper eigenvalues of MV_1M w.r.t. MV_2M (see Rao and Mitra (1971, Section 6.3). Here r is the rank of MV_2M. Some of the λ_i's could be zero and some of them may be repeated.

<u>Corollary 2</u> Let $k=2$ in model (I) and suppose V_1 and V_2 are nnd. Let $\lambda_i (i=1,2,\dots,r)$ be as defined above.

(a) Suppose $R(MV_1M) \cap R(MV_2M) = \{0\}$. If MV_1M and MV_2M are nonnull, then $q'\theta$ is nonnegatively estimable iff $q_1 \geq 0$, $q_2 \geq 0$.

(b) Suppose $R(MV_1M) \cap R(MV_2M) \neq \{0\}$. Then

(i) if $R(MV_1M) \not\subset R(MV_2M)$, $q'\theta$ is nonnegatively estimable iff $q_1 \geq q_2\lambda_r \geq 0$.

(ii) If $R(MV_1M) \subset R(MV_2M)$ and $\text{rank}(MV_1M) < \text{rank}(MV_2M)$, then $q'\theta$ is nonnegatively estimable iff $q_2\lambda_1 \geq q_1 \geq 0$.

(iii) If $R(MV_1M) = R(MV_2M)$, then $q'\theta$ is nonnegatively estimable iff $q_2\lambda_1 \geq q_1 \geq q_2\lambda_r \geq 0$.

<u>Proof</u>: Since V_1 and V_2 are nnd, any nonnegatively estimable $q'\theta$ must have $q_1 \geq 0$, $q_2 \geq 0$ (LaMotte, 1973). Using Theorem 6.3.4 in Rao and Mitra (1971), we see that there exists a nonsingular matrix P satisfying $P'MV_2MP = \text{diag}(I_r,0)$ and $P'MV_1MP = \text{diag}(\Lambda_1,\Lambda_2)$ where $\Lambda_1 = \text{diag}(\lambda_1,\lambda_2,\dots,\lambda_r)$ and $\Lambda_2 = \text{diag}(\lambda_{r+1},\dots,\lambda_n)$.

(a) $R(MV_1M) \cap R(MV_2M) = \{0\}$ iff $\Lambda_1 = 0$. In such a case, for $q_1 \geq 0$, $q_2 \geq 0$, $\frac{q_1}{\text{rank}(\Lambda_2)} Y'P \operatorname{diag}(0, \Lambda_2^+)P'Y + \frac{q_2}{r} Y'P \operatorname{diag}(I_r, 0)P'Y$ is an nnd unbiased estimator of $q'\theta$.

(b) $MV_qM = P'^{-1}\operatorname{diag}(\lambda_1 q_1 + q_2, \ldots, \lambda_r q_1 + q_2, q_1\lambda_{r+1}, \ldots, q_1\lambda_n)$ and $MV_1M - q_1MV_qM = q_2P'^{-1}$ $\operatorname{diag}(q_2\lambda_1 - q_1, \ldots, q_2\lambda_r - q_1, q_2\lambda_{r+1}, \ldots, q_2\lambda_n)$ (using the assumption $q_1^2 + q_2^2 = 1$). If q_1 or q_2 is zero, then it can be verified that the necessary and sufficient condition for the nonnegative estimability of a single variance component as given in Theorem 5.1 of Pukelsheim (1977) or Theorem 3 in Kleffe (1977) or Theorem 5.5.1 in Rao and Kleffe (1980) reduce to those given in the theorem. We now consider the case $q_1 \neq 0$, $q_2 \neq 0$.

(i) When $R(MV_1M) \not\subset R(MV_2M)$, $\Lambda_2 \neq 0$. Let us assume $\lambda_{r+1} > 0$, If $q_2\lambda_r - q_1 > 0$, then $MV_1M - q_1MV_qM$ is nnd and has the same range as MV_qM. Hence from Corollary 1(ii) it follows that $q'\theta$ is not nonnegatively estimable. Conversely, if $q_2\lambda_r - q_1 \leq 0$, since $\lambda_{r+1} > 0$ and $MV_qM \geq 0$, we can find an nnd A satisfying $\operatorname{tr} AMV_qM > 0$ and $\operatorname{tr} A(MV_1M - q_1MV_qM) = 0$. Then $\frac{1}{\operatorname{tr} AMV_qM} Y'MAMY$ is an nnd unbiased estimator of $q'\theta$. We observe that $R(MV_1M) \subset R(MV_2M)$ iff $\Lambda_2 = 0$ and then rank $(MV_1M) <$ rank(MV_2M) iff $\lambda_r = 0$. Using these observations, the rest of the corollary can be established using Corollary 1. □

. Corollary 2 reduces to Theorem 1 in Baksalary and Molinska (1984) when $V_2 = I$.

Let V_0 be the nnd matrix as defined in assumption 3. Let U_0 be an nnd matrix satisfying $MV_0MU_0 = 0$ and $MV_0M + U_0$ is p.d.

<u>Theorem 2</u>. Suppose $(I-P_q)MV_qM(I-P_q)$ is a nonnull nnd matrix of rank r_0. Then

(i) the estimator $\frac{1}{r_0} Y'[(I-P_q)MV_qM(I-P_q)]^+Y$ is an nnd unbiased estimator of $q'\theta$.

(ii) if there exists an nnd matrix W_0 as specified in Theorem 1 (ii), the above estimator is the MINQUE$(MV_0M+U_0$, NND) of $q'\theta$.

Proof: (i) We observe that $\mathrm{tr}[((I-P_q)MV_qM(I-P_q)]^+(V_i-q_iV_q) = 0$ for $i = 1,2,\ldots,k-1$ and $\mathrm{tr}[(I-P_q)MV_qM(I-P_q)]^+V_q = \mathrm{tr}[(I-P_q)MV_qM(I-P_q)]^+[(I-P_q)MV_qM(I-P_q)] = \mathrm{rank}[(I-P_q)MV_qM(I-P_q)]$. Thus, the estimator given in the theorem is an nnd unbiased estimator of η_k in (II) and hence that of $q'\theta$ in (I).

(ii) Let $Y'B_*Y$ denote the nnd estimator of $q'\theta$ given in part (i) of the theorem and let $Y'BY$ be any other nnd unbiased estimator of $q'\theta$. We first show that $B = (I-P_q)MBM(I-P_q)$ when there exists a matrix W_0 as specified in Theorem 1 (ii). The matrix B satisfies $BX = 0$, $\mathrm{tr}\, BV_q = 1$ and $\mathrm{tr}\, B(V_i-q_iV_q) = 0$ $(i = 1,2,\ldots,k-1)$. Since $BX = 0$ iff $B = MBM$, the last set of conditions give $\mathrm{tr}\, B(MV_iM-q_iMV_qM) = 0$ $(i = 1,2,\ldots,k-1)$, which implies $\mathrm{tr}\, BW_0 = 0$ or equivalently $BW_0 = 0$. Thus B satisfies $BX = 0$, $B(MV_iM-q_iMV_qM) = 0$ and hence $B = (I-P_q)MBM(I-P_q)$. Now let $\|B\|_0^2 = \mathrm{tr}\, B(MV_0M+U_0)B(MV_0M+U_0) = \|B_*\|_0^2 + \|B-B_*\|_0^2 + 2\,\mathrm{tr}\, B_*(MV_0M+U_0)(B-B_*)(MV_0M+U_0) = \|B_*\|_0^2 + \|B-B_*\|_0^2 + 2\,\mathrm{tr}\, B_*MV_0M(B-B_*)MV_0M$. The proof is complete if we show that the last term is zero. Since $V_0 \in \mathrm{sp}\{V_1,V_2,\ldots,V_k\} = \mathrm{sp}\{V_q,V_1-q_1V_q,\ldots,V_{k-1}-q_{k-1}V_q\}$, $V_0 = \alpha_1V_q + \sum_{i=1}^{k-1}\alpha_i(V_i-q_iV_q)$, where $\alpha_1 \neq 0$ (since $(I-P_q)MV_qM(I-P_q) \neq 0$). Then $\mathrm{tr}\, B_*MV_0M(B-B_*)MV_0M = \alpha_1^2(\mathrm{tr}B_*MV_qM(B-B_*)MV_qM$ and $\mathrm{tr}B_*MV_qMBMV_qM = \mathrm{tr}B_*(I-P_q)MV_qM(I-P_q)MBM(I-P_q)MV_qM(I-P_q) = \frac{1}{r_0}\,\mathrm{tr}(I-P_q)MV_qM(I-P_q)MBM = \frac{1}{r_0}\,\mathrm{tr}\, BV_q = \frac{1}{r_0} = \mathrm{tr}\, B_*MV_qMB_*MV_qM$. □

Remark 3. If we are interested in the nonnegative estimability of a single variance component, Theorem 2 (ii) reduces to Theorem 5.5.2 in Rao and Kleffe (1980) when the matrices V_i $(i = 1,2,\ldots,k)$ in (I) are nnd.

As an example, we consider a model with two variance components $Y \sim (X\beta, \sigma_1^2 I_b \otimes 1_k1_k' + \sigma_2^2 I_b \otimes I_k)$ where 1_k is a k-component vector of ones, $\sigma_1^2 \geq 0$, $\sigma_2^2 \geq 0$. Such a model arises in the interblock analysis of a block design with b blocks, each block having k plots. A model from genetics discussed by Gnot and Kleffe (1983, p. 275) is also of the above form. An explicit characterization of q_1

and q_2 such that $q_1\sigma_1^2 + q_2\sigma_2^2$ is nonnegatively estimable can be obtained using Corollary 2 or Theorem 1 in Baksalary and Molinska (1984). We shall consider the nonnegative estimation of σ_2^2 and $(k\sigma_1^2+\sigma_2^2)$. These are the parametric functions of interest when we want to combine the inter and intra block estimates of the treatment contrasts in a block design. For the estimation of σ_2^2, Theorem 1 (ii) and Theorem 2 (ii) clearly applies. Let $M = I - XX^+$, $V_1 = I_b \otimes 1_k 1_k'$, $V_2 = I_b \otimes I_k$, $q_1 = \frac{k}{\sqrt{1+k^2}}$ and $q_2 = \frac{1}{\sqrt{1+k^2}}$. Then $V_q = \frac{1}{\sqrt{1+k^2}}(kV_1+V_2)$ and $V_1-q_1V_q = \frac{1}{1+k^2}(V_1-kV_2)$. Since $V_1-q_1V_q$ is nonpositive definite, so is $MV_1M-q_1MV_qM$. Thus the nonnegative estimability of $k\sigma_1^2+\sigma_2^2$ can be verified using Theorem 1 (ii). When it is nonnegatively estimable (which is the case for a block design) its MINQUE (I, NND) can be computed using Theorem 2 (ii). Explicit characterization of nonnegatively estimable $q'\theta$ for some ANOVA models is given in Pukelsheim (1979, 1981a).

4. Characterization of Nonnegative Estimability using MINQUE.

We now proceed to obtain conditions under which MINQUE (given Σ) characterizes nonnegative estimability in model (I).

Let $\mathcal{B}$ be a subspace of real symmetric matrices of order n. For an n×n positive definite matrix N, let P_N denote the orthogonal projector onto $\mathcal{B}$, where orthogonality is w.r.t. the inner product $\langle A,B\rangle = \text{tr } ANBN$; A,B symmetric.

Definition 3. We say that $\mathcal{B}$ is an N-quadratic subspace if $BNB \in \mathcal{B}$ whenever $B \in \mathcal{B}$.

Definition 4. We say that $\mathcal{B}$ preserves nonnegative definiteness wr.r.t. N if $P_N(B) \geq 0$ whenever $B \geq 0$.

Definition 3 is given in Musiela and Zmyslony (1978, Appendix). Definition 4 is a generalization of a definition given in Mathew (1984) and is a special case of the definition of a nonnegativity preserving linear transformation given in

de Pillis (1967). It is clear that $\mathcal{B}$ preserves nonnegative definiteness w.r.t N iff $N^{1/2}\mathcal{B}N^{1/2} = \{N^{1/2}BN^{1/2} : B \in \mathcal{B}\}$ preserves nonnegative definiteness w.r.t. I. Using this observation characterization of subspaces that preserve nonnegative definiteness can be obtained similar to Lemma 1 and Lemma 2 in Mathew (1984). It can also be shown that an N-quadratic subspace preserves nonnegative definiteness w.r.t. N, (cf. Pukelsheim 1981a, Lemma 2).

Let M_Σ be as defined in section 2 and let $\mathcal{B}_\Sigma$ denote the subspace spanned by the matrices $M_\Sigma V_i M_\Sigma'$ $(i = 1,2,\ldots,k)$. The following result is a generalization of Theorem 2 in Pukelsheim (1981a) and the theorem in Mathew (1984).

Theorem 3. (i) MINQUE (given Σ) characterizes nonnegative estimability in (I) iff $\mathcal{B}_\Sigma$ preserves nonnegative definiteness w.r.t. Σ^{-1}.

(ii) Let $\mathcal{B}_\Sigma$ preserve nonnegative definiteness w.r.t. Σ^{-1} and suppose $\mathcal{B}_\Sigma$ is k-dimensional. Then $\sum_{i=1}^{k} \hat{\theta}_i M_\Sigma V_i M_\Sigma'$ is nnd, where $\hat{\theta}_i$ denotes the MINQUE (given Σ) of θ_i.

The theorem follows from the corresponding results for the case $\Sigma = I$ once it is observed that MINQUE (given Σ) characterizes nonnegative estimability in (I) iff MINQUE (given I) characterizes nonnegative estimability in the model $\Sigma^{-1/2}Y \sim (\Sigma^{-1/2}X\beta, \Sigma^{-1/2}V_\theta\Sigma^{-1/2})$.

In the introduction, it has been pointed out that MINQUE (given I) always characterizes nonnegative estimability in a general m-way classification model with balanced data. We shall now apply the reuslts in this section to the multivariate linear model $Y \sim ((I_p \otimes X)\beta,\ \ddagger \otimes V)$, where $\ddagger$ of order p is unknown and V is a known nnd matrix. Let U be an nnd matrix satisfying $(V+XX')U = 0$ and $G = V+XX'+U$ is p.d. Let $M_G = I - X(X'G^{-1}X)^{-}X'G^{-1}$. Then subspace $\mathcal{B}_{I\otimes G}$ consisting of matrices $S \otimes M_G V M_G'$ is an $I \otimes G^{-1}$-quadratic subspace of dimension $\frac{p(p+1)}{2}$, where S is any symmetric matrix of order p. Hence for checking the nonnegative estimability of a linear combination of the components of $\ddagger$, it is enough to check the nonnegativity of its MINQUE (given $I\otimes G^{-1}$). Furthermore, the estimate of $\ddagger$ obtained from the

MINQUE (given $I \otimes G^{-1}$) of its components is nnd. For the case $V = I$, these observations are given in Pukelsheim (1981a, p. 295).

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